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Basic Modeling of Openness, Quantum States and Transport in Two- and Three-Dimensional Ballistic Cavities

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A basic model for particle states and current flow in open quantum dots/billiards are investigated. The model is unconventional and extends the use of complex potentials first introduced in phenomenological nuclear inelastic scattering theory (the optical model). Attached leads/source drain are represented by complex potentials. Probability densities and currents flows for open 2D quantum dots/billiards are calculated and the results are compared with microwave measurements used to emulate the dot. We also apply the model to a rectangular enclosure and report on helical flows guided by nodal lines and disc-like accumulations of flow lines. The model is of conceptual as well as practical and educational interest

Keywords: nano-scale systems, quantum dots, microwave billiards, quantum transport, vortices, helical motion, streamlines.

Introduction

Due to advances in semiconductor technology it is now possible to fabricate high-quality modulation doped layered materials in which electrons form a two-dimensional high-mobilty electron gas at the interface of the two materials, typically $\mathrm{Al_xGa_{1-x}As/GaAs}$ (see, for example, [1]). By lithographic patterning together with suitably located gates and application of external voltages it is possible to "electrostatically squeeze" the electron gas into a varity of nano-sized closed structures. If they are sufficiently small the electrons inside such confinements occupy discrete quantized states. Simple examples of "quantum dots" or "billiards" of this kind are squares, rectangles and circular discs in which the motion is regular. Arbitrarily shaped cavities with irregular dynamics may also be fabricated, for example, in the shape of a stadium. The flexibilty of this type of systems is of obvious interest for studies of statistical properties of quantum states and related cross-over phenomena. Quantum dots may be closed or open. Openness implies that there are attached leads by which a current may be passed through a dot. If the nominal mean free path exceeds the dimensions of a dot the transport is ballisitic. An example of a square dot is shown in Fig. 1 for a realistic case (a $\mathrm{Al_xGa_{1-x}As/GaAs}$ heterojunction with a patterned metallic gate). It is rewarding that quantum dots as in Fig. 1 may be emulated by planar microwave resonators [2,3]. In the case of independent electrons "macroscopic wave functions", currents etc may be obtained from measurements as will be briefly below. RLC electrical networks are other examples of classical analogue systems [4].

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Because of the current scientific/technological focus on quantum dots and cavities it is of interest to model electron states, transport etc. There are many ways to do this but here we will present a basic heuristic model that extends ideas originally developed for inelastic scattering in nuclear physics [5, 6]. In a way it is a "light version" of more rigorous methods to introduce openness into nominally closed cavities by means of an effective non-Hermitian Hamiltonian (see, e.g., [7, 8] and refs. within). The model is easy to implement and, additionally, it should be of educational interest for introductory courses on quantum mechanics. Already at an early stage of their education students may get their hands on how to model realistic systems of current scientific and technological interest like open quantum dots, etc.

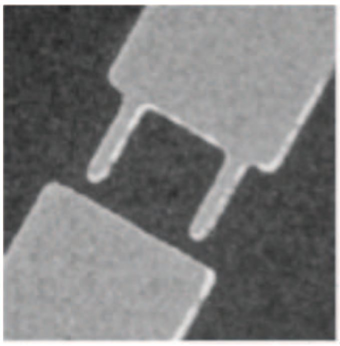

Fig. 1. Scanning electron micrograph of a gated two-dimensional square quantum dot with dimensions $1\times 1\mu m^2$ (middle dark region). The dot is connected to surrounding electron reservoirs (outer dark areas) by two openings (leads) through which an electric current may be passed from one reservoir to the other by applying a driving voltage between the resevoirs. Regions in light gray are patterened metallic gates under which the electron gas is depleted. (Adapted from [9], courtesy J.P. Bird)

Here we want to show how knowledge on this level is sufficient for modeling wave functions and quantum transport in quantum dots and cavities with leads for input and output of a current. With other words we will be able to address problems of much current scientific and technological interest (see, for example, [1]).

1. Quantum Mechanics with Complex Potentials

Consider the usual time-dependent Schrödinger equation

$$i\hbar\partial\Psi(\mathbf{r},t)/\partial t = -\frac{\hbar^2}{2m}\Delta\Psi(\mathbf{r},t) + V\Psi(\mathbf{r},t); \tag{1}$$

where V is the potential and m the (effective) mass of the particle. Then the probability current density $\mathbf{J}$ is

$$\mathbf{J} = \frac{\hbar}{2mi}[\Psi^*\nabla\Psi - (\nabla\Psi^*)\Psi] \tag{2}$$

The continuity equation relates $\mathbf{J}(\mathbf{r},t)$ to the probabilty density $\varrho(\mathbf{r},t) = |\Psi(\mathbf{r},t)|^2$ as

$$\partial\varrho/\partial t + \nabla\cdot\mathbf{J} = 0. \tag{3}$$

For stationary states the Schrödinger equation in Eq. (1) turns into

$$-\frac{\hbar^2}{2m}\Delta\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{4}$$

where E is the energy of the particle. For the following arguments let $\Psi(\mathbf{r},t) \to \psi(\mathbf{r})exp(-iEt/\hbar)$, $\mathbf{J}(\mathbf{r},t) \to \mathbf{j}(\mathbf{r})$ and $\varrho(\mathbf{r},t) \to \rho(\mathbf{r})$.

According to Eq. (3) there is a differential conservation relation between $\varrho(\mathbf{r},t)$ and the probability $\mathbf{J}(\mathbf{r},t)$. A prerequisite is that the potential V is real. The idea of using a complex potential was, as mentioned above, introduced long ago in a phenomenological model for describing absorption in nuclear scattering [5, 6], i.e. in situations when particle conservation is not mandatory. The model with complex V, also referred to as the optical model, is indeed an heuristic one and as such frequently used in nuclear physics as well as in other fields like atomic and molecular physics, nanotransport etc to describe inelastic losses. In the present context we may specifically mention the modeling of electron wave patterns in "quantum corrals" or "ringed electrons" and the reduced reflectivity of their surrounding walls of iron atoms [10] and studies of electron transport of quantal trajectories and dephasing in two-dimensional nano-devices [11,12].

Assume now that V is complex and is written as

$$V = V_R + iV_I, \tag{5}$$

where V_R and V_I are real. Eq. (3) then turns into

$$\partial\varrho(\mathbf{r},t)/\partial t + \nabla\cdot\mathbf{J}(\mathbf{r},t) = \frac{2V_I}{\hbar}\varrho(\mathbf{r},t). \tag{6}$$

The term on the right hand side acts as source or sink for positive or negative values of V_I, respectively. In general the eigenvalues are now complex and there is either an exponential growth or decay depending on the sign of V_I.

The idea here is to combine the two cases to study probability current flow, vortices etc. by letting V_I have different signs in different parts of the system. For example, to simulate the probability current density flowing between input and output leads in an open cavity like the one in Fig. 1 we may simply replace leads/reservoirs by two regions in which V_I is non zero and of opposite signs. The condition for a steady well-balanced and lossless flow between the two regions is

$$< V_I >= \int_\Omega V_I\varrho(\mathbf{r},t)d\mathbf{r} = 0. \tag{7}$$

Therefore the expectation value of the Hamiltonian operator, $< H >$, is real in spite of $V = V_R + iV_I$ being complex. Furthermore, the corresponding eigenvalues are real when V_R is independent of time. As we will see in below our elementary approach of using $\pm iV_I$ for source and sink to emulate probability distributions for ρ and $\mathbf{j}$ within a cavity performs remarkably well and may therefore serve as a first useful guide to such features.

2. Solutions for an Open Two-Dimensional Quantum Dot

Fig. 2 illustrates how extended leads may be replaced by short stubs and source and drain by regions of complex V for the case of an open dot as in Fig. 1. Because of previous modeling work as well as available experimental data we have chosen to simulate this particular device [9,17,18].

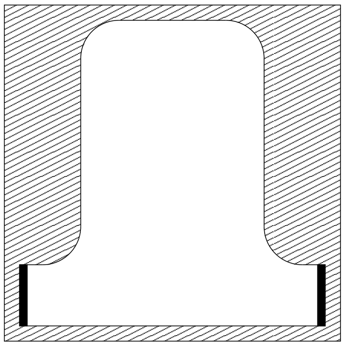

Fig. 2. Modeling of a "two leads" quantum dot for which the leads are replaced by stubs (cf Fig. 1). Sharp corners have been rounded because of electrostatic smearing at the interface [9]. The systen is thus akin to an open semi-stadium. Inside the dot (including the stubs) the real part $V_R = 0$; in the exterior shaded areas V_R should be given a value that is much higher than the levels one wishes to compute. The dark areas at the two ends of the stubs indicate the location for source and sink ($\pm iV_I$)

Systems for which one may find analytical solutions to the Schrödinger equation with complex potential V are rare. For realistic devices as here one must resort to numerical methods, for example, the finite difference method (FDM) for stationary states that to be used here. There are also other efficient numerical methods like the finite element method (FEM), Green function techniques etc. Here we prefer to use FDM as it is robust and straightforward to implement and, once wave functions are known, it is easy to evaluate related quantities like the probability current density as well as other features like statistical distributions and correlations. FDM may also be extended into the time domain (finite-difference time-domain FDTD) for studies of time-dependent processes. For weakly open systems a combination of FDM for the closed systems and 2nd order perturbation theory for V_I performs quite well.

When solving for the wave functions and eigenvalues for the device in Fig. 2 we choose Dirichlet boundary conditions except for the two vertical ends of the stubs at which Neumann boundary conditions appear more natural as we wish to emulate extended leads and particle flow. In practice this point is, however, not crucial. Fig. 3 shows the simulated probability densities, $\rho(x, y) = |\psi(x, y)|^2$ and probabilities current flow $\mathbf{j}(x, y)$ for a typical case. To avoid a mixing of adjacent states as V_I is turned on one should choose V_I less than the spacing between the energy levels of the corresponding closed system. Besides this restriction, however, the actual value of V_I is not crucial in the present context. (The mixing of levels because of V_I is, of course, an important problem on its own right.) With such a choice the system is weakly open. (For a rough estimate one may use the level spacing in rectangular box.) Furthermore we let the two regions in which V_I is finite be symmetrically located as in Fig. 2 with $V_I(x, y) = -V_I(-x, y)$. Therefore $< V_I >$ in practice vanishes because $\varrho(x, y)$ is symmetric for our type of systems as long as V_I is chosen small. As a consequence the eigenvalues become real to very high degree of accuracy and the corresponding states may therefore be regarded as stationary.

Because V_I is chosen small the densitiy $\rho(x, y)$ in Fig. 3 is very similar the case of the closed dot. The figure also clearly shows how a current flow from one lead to the other is set up. Because of the smallness of V_I the net current is also small. At the same time as net currents may be small local currents may be significant in any part of the cavities as in the case displayed. Typically

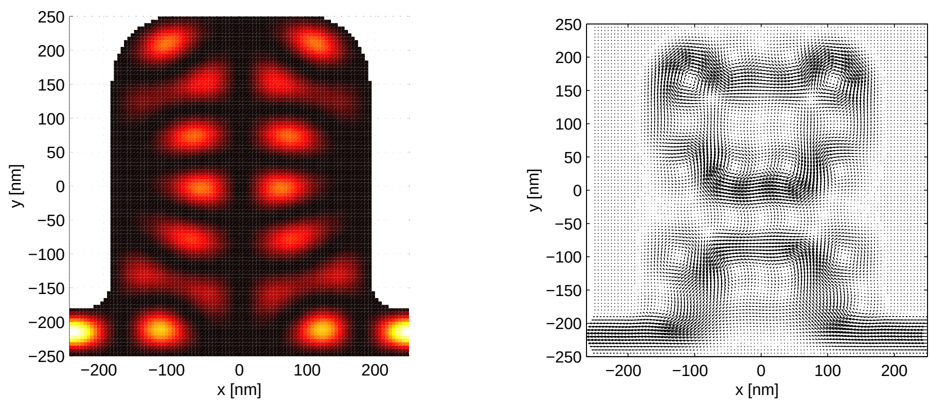

Fig. 3. Probability density $\rho(x, y)$ (left panel) and probability current flow $\mathbf{j}(x, y)$ (right panel) as obtained from simulations ($E = 1.251\ meV$; effective mass $m_{GaAs} = 0.067 m_e$) [13]. Dark and light areas in the density plot correspond to low and high densities, respectively. The state is reminiscent of a "particle-in-a box" state with $n_x = 2$ and $n_y = 7$ that is distorted by the leads and rounded corners. The accumulation of density in the leads tells that the cavity is quite open

there are vortices centered at the nodal points where $\psi(x, y)$ vanishes. The vortex currents tend to integrate to zero and, if any at all, normally gives only small contributions to the net current through the cavity.

For higher energies the solutions become increasingly complex/chaotic. For such states the model yields good agreement [13] with the analytic statistical distributions for vortices [14], ρ, $\mathbf{j}, j_x, j_y$ [15] and the stress stensor components $\sigma_{\alpha\beta}$ [16].

3. Experimental Studies of a Planar Microwave Analog

As indicated above quantum dots may be emulated by planar micro wave resonators [2, 3]. Thus there is a one-to-one correspondence between the TM modes of the electromagnetic field and the wave functions of the corresponding quantum system. The z-component of the electromagnetic field E_z, perpendicular to the planar resonator, then corresponds to the quantum-mechanical wave function ψ and obeys the Helmholtz equation which in this case is identical to the Schrödinger equation for a particle in a hard-wall dot. The Poynting vector is the analogue to the quantum-mechanical probability current density. The wave number for the microwave is $k = \omega/c$ where ω is the angular frequency of the TM mode and c the speed of light.

Microwave measurements are available for a number of cavity of different shapes [3]. In particular there are early measurements [17, 18] designed to record the wave function analogs in resonators exactly shaped as the quantum dot in Figs. 1 and 2 (cf ref. [9]). The dimensions of the planar resonator are $(16 \times 21)\ cm^2$ and the width of the two attached leads is 3 cm, i.e. there is simply a scale up of our quantum billiard to the macroscopic world. Antennas placed in the leads as in Fig. 4 act as source and drain for the microwaves. The field distribution inside the cavity has been obtained via a probe antenna moved on the grid indicated in Figs. 4. The absorption through this third antenna may normally be made small and for such cases it may be disregarded in the data analysis. In contrast to the quantum mechanical case one may thus measure the emulated "wave function", its amplitude as well as its phase. Having

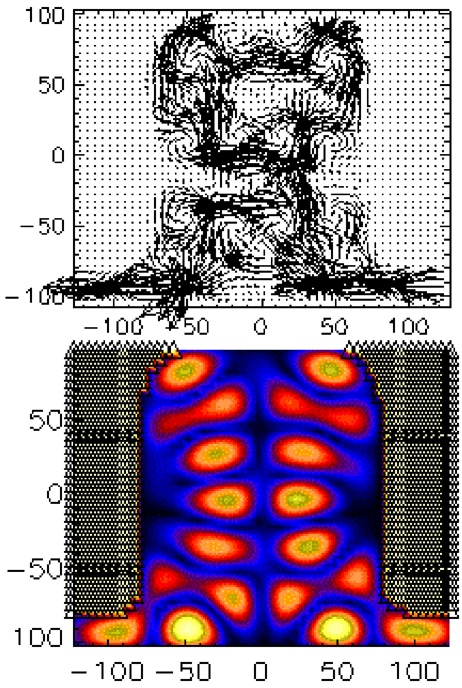

Fig. 4. Probability current flow (upper case) and probability density (lower case) as obtained from microwave measurements at 5.403 GHz [17] to be compared with simulations in Fig. 3. Dark and light areas in the density plot correspond to low and high densities, respectively. The numbering on the $x-$ and $y-$axes define grid points (Courtesy M. Barth)

this information one may evaluate the density distribution and the emulated probability current density shown in Fig. 4 for a case chosen to match Fig. 3. The overall agreement between the two graphs, together with similar results for a number of other energies, tells that the present model with positive and negative imaginary potentials for source and drain in open quantum dots/billiards yields realistic results.

4. Open Three-Dimensional Quantum Dots

Compared to the 2D case wave function form and flow patterns in open 3D dots and cavities appear to be much less explored. Computations and measurements as above generally tend to be much more tedious or even impractical. Here we will present the results for an open rectangular quantum box. Although this example is quite elementary it reveals fascinating generic 3D flow patterns that appear to have passed unnoticed so far (for a first account based on the Berry function, see [19]).

In the 2D case vortices are formed around the nodal points of a complex wave function. The vortical motion is either clockwise or counter-clockwise. To analyze the corresponding features in the 3D case we apply the same modeling as for the 2D case above, i.e. we introduce imaginary terms to mimic source and drain. Rather than making use of numerical FDM solutions, which would generally be computationally quite heavy, we may use the analytic "particle-in-a-box" for the closed rectangular dot in combination with second order perturbation theory to account for "imaginary inclusions $\pm iV_I$", for example located at the cornes of the box.

In 3D the nodal points typical for 2D are replaced by nodal lines that are defined as the intersection between the real and imaginary parts of the wave function. Typical results for the interwiding 3D nodal lines at which $Re(\psi) = Im(\psi) = 0$ are shown in Fig. 5 as solid lines. The 3D case is evidently much more complex and, as indicated already, it is not immediately clear how to find a structure among all the entangled nodal lines. However, streamlines are most useful in this respect. By tracing a set of trial streamlines one basically finds that the vortices that are typical for 2D evolve in 3D into left- or right-handed helical motions guided by the different nodal lines.

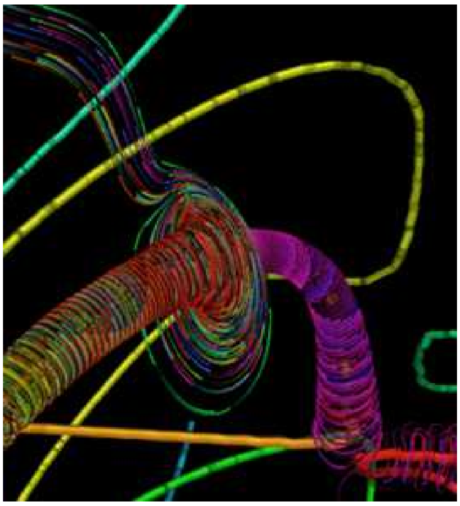

Fig. 5. Incoming streamlines forming a rotational disc-like object from which spiraling streamlines, guided by a selected nodal line, emerge in opposite directions. For clarity other streamlines are not shown here

There is also another interesting difference from 2D systems in which streamlines encircling the different nodal points remain closed, i.e. they are "tied to" the vortex. In 3D, on the other hand, there are crossovers from one line to another frequently take place when nodal lines get close to each other. A streamline may thus successively "jump from nodal line to nodal line". By selective tracing one finds even more intriguing "disc"-like or "galaxy"-like accumulations of streamlines as illustrated by Fig. 5. As seen there are incoming streamlines that first merge to create a rotational disc which subsequently splits into helices progressing in opposite directions but with the same helicity. Assume that this happens on a closed nodal line. The two helical streamlines emerging from the disc will then have to meet somewhere on the loop, but can only do so by forming another disc from which the streamlines eventually ejected and spread into other more remote parts of the system. This process may take place many times on the closed loop but there must be an even number of discs and the helicity must be conserved along the loop.

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Моделирование незамкнутости, квантовых состояний и транспорта в двух- и трехмерных баллистических резонаторах

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Ирина И. Якименко

В работе исследуется базовая модель для состояния частицы и токового потока в открытом квантовом биллиарде/резонаторе. Предложенная модель обобщает подход комплексного потенциала, который был впервые введен в ядерной физике для феноменологического описания неэластичных процессов рассеяния (так называемая оптическая модель). Прикрепленные к резонатору контакты представлены комплексным потенциалом. Мы рассчитываем плотность вероятности и линии тока и сравниваем результат с экспериментальными результатами для микроволновых биллиардов, имитирующими квантовые резонаторы. Мы также применили модель к прямоугольному трехмерному резонатору и обнаружили спиральные потоки вдоль нодальных линий и дискообразную аккумуляцию линий тока. Модель является концепцуальной, практической и интересной с образовательной точки зрения.

Ключевые слова: наносистемы, квантовые точки, микроволновые биллиарды, квантовый транспорт, вихри, спиральное движение, линии тока.